

**Procedures for Addressing Uncertainty and
Variability in Exposure to Characterize
Potential Health Risk From Trichloroethylene
Contaminated Groundwater at Beale Air Force
Base in California**

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PREFACE

This study was designed to accomplish two objectives. The first was to provide to the US Air Force and the regulatory community quantitative procedures that they might want to consider using for addressing uncertainty and variability in exposure to better characterize potential health risk. Such methods could be used at sites where populations may now or in the future be faced with using groundwater contaminated with low concentrations of the chemical trichloroethylene (TCE). The second was to illustrate and explain the application of these procedures with respect to available data for TCE in ground water beneath an inactive landfill site that is undergoing remediation at Beale Air Force Base in California. The results from this illustration provide more detail than the more traditional conservative deterministic, screening-level calculations of risk, also computed for purposes of comparison. Application of the procedures described in this report can lead to more reasonable and equitable risk-acceptability criteria for potentially exposed populations at specific sites.

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ABSTRACT

Conservative deterministic, screening-level calculations of exposure and risk commonly are used in quantitative assessments of potential human-health consequences from contaminants in environmental media. However, these calculations generally are based on multiple upper-bound point estimates of input parameters, particularly for exposure attributes, and can therefore produce results for decision makers that actually overstate the need for costly remediation. Alternatively, a more informative and quantitative characterization of health risk can be obtained by quantifying uncertainty and variability in exposure. This process is illustrated in this report for a hypothetical population at a specific site at Beale Air Force Base in California, where there is trichloroethylene (TCE) contaminated ground water and a potential for its future residential use. When uncertainty and variability in exposure were addressed jointly for this case, the 95th-percentile upper-bound value of individual excess lifetime cancer risk was a factor approaching 10 lower than the most conservative deterministic estimate. Additionally, the probability of more than zero additional cases of cancer can be estimated, and in this case it is less than 0.5 for a hypothetical future residential population of up to 26,900 individuals present for any 7.6-y interval of a 70-y time period. Clearly, the results from application of this probabilistic approach can provide reasonable and equitable risk-acceptability criteria for a contaminated site.

INTRODUCTION

Quantitative assessments of the potential human health risks from contaminants present at hazardous-waste sites typically involve conservative deterministic, screening-level calculations of exposure and risk, often based on multiple upper-bound point estimates of input parameters. Because inherent conservatism in such estimates may result in highly inefficient strategies for site cleanup, there is growing interest in obtaining more informative and quantitative characterizations of human-health risk (NRC, 1994). Such assessments require quantitative methods to characterize joint uncertainty and interindividual variability (JUV) in estimated risk, based on both uncertainty and/or interindividual variability reflected in each input parameter (Bogen and Spear, 1987; NRC, 1994; Bogen, 1995). Uncertainty here refers to an absence of measurement data or incomplete knowledge; interindividual variability (or "variability") here refers to true differences or heterogeneity in an empirical, risk-related characteristic (e.g., physiological differences) among individuals in a population (Bogen and Spear, 1987). Such probabilistic assessments can be resource intensive, but are generally appropriate at sites for which deterministic upper-bound calculations of risk overstate the need for costly remediation efforts. A glossary of the important terms associated with the JUV analysis procedures described in this report is presented in Appendix A.

This report provides a site-specific illustration of how JUV in exposure may be used to characterize risk. Results from such analyses provide an improved understanding of risk for decision makers, including estimates of the upper-bound risk to the average person in the population, the risk to an individual at the upper-bound of exposure, and the likelihood of additional cases of cancer in a population exposed to low-level site contaminants. The case study addresses inactive Landfill Site LF-13 on

Beale Air Force Base in California, where groundwater contaminated with trichloroethylene (TCE) has moved beyond the site boundary. Consequently, soil-vapor extraction and air-stripping treatment of groundwater have been undertaken at Site LF-13 to remediate this situation (URSGWC, 1998). Specifically, these actions are designed to reduce to low-levels the concentrations of TCE (and other volatile organic compounds) in the ground water beneath Site LF-13. This is especially important because in this currently rural area of the Sacramento Valley of California, groundwater wells are the principle source of domestic-water supplies. Thus, elevated levels of TCE contamination, particularly, would prevent this water from being used for this purpose. Accordingly, this analysis focuses on potential risks attributable to a scenario that theoretically could involve possible future domestic, residential uses of groundwater from beneath Site LF-13 that contains residual, low-level concentrations of TCE. This scenario is considered appropriate for addressing hypothetical residential populations of different sizes that might eventually occupy lands adjacent to the site. The measurements of TCE-concentration used for this analysis were those obtained in 1997 from the groundwater monitoring well on Site LF-13 near the possible location of a future groundwater extraction and distribution system (Purrier, 1997). A characterization of JUV in risk is performed, and corresponding estimates of the expected number of additional cancer cases and the probability of greater than zero additional cases for specified populations are obtained. Finally, risk estimators from the JUV approach are compared to those calculated using the traditional framework for computing risk deterministically.

METHODS

The procedures utilized here are ones designed to address JUV in the context of risk characterization (Bogen and Spear, 1987; NRC, 1994; Bogen, 1995). For TCE in groundwater at Site LF-13 on Beale Air Force Base in California, total risk, R , is defined as the increased lifetime probability of cancer for an individual attributable to TCE exposure from three pathways: direct ingestion, E_{Ing} , of TCE-contaminated groundwater; dermal absorption, E_{Derm} , of TCE while showering or bathing; and inhalation, E_{Inh} , of TCE volatilized from water to household air. For volatile organic compounds such as TCE, these three pathways typically are the most significant contributors to its total daily dose (or intake).

This document uses a consistent approach that conforms with previous application of JUV notation (see also the glossary of important terms appearing in Appendix A): an overbar (i.e., $\overline{}$) is used to denote expectation with respect to heterogeneous parameters only, and angle brackets (i.e., $\langle \rangle$) to denote expectation with respect to uncertain parameters only (Bogen and Spear, 1987; NRC, 1994; Bogen, 1995). A tilde (i.e., \sim) appearing over a term shall be used to denote a sample mean of empirical values.

Exposure-Pathway Models

The three equations described next are used to model the most important human-exposure pathways for TCE in ground water. These equations are consistent with those described by USEPA (1989) and also CalEPA/DTSC (1994) for modeling these exposure pathways.

Exposure to TCE from direct ingestion of groundwater was calculated using Eq. 1.

$$E_{\text{ing}} = \text{Ing} \times ED \times \frac{EF}{AT} \times C_w, \quad (1)$$

where

E_{ing} = TCE-exposure (intake) resulting from direct ingestion of contaminated ground water [mg/(kg-d)];

Ing = daily water ingestion rate per unit body weight [L/(kg-d)];

ED = exposure duration, also referred to as time of residence (y);

EF = exposure frequency (d/y);

AT = averaging time corresponding to a 70-y lifetime of exposure (d); and

C_w = TCE concentration in ground water (mg/L).

TCE can volatilize to indoor air from water used in showering, bathing, and by the use of toilets, dishwashers, washing machines, and cooking. Inhalation exposure to TCE was calculated by the procedure of McKone and Bogen (1992) for estimating uptake of a volatile contaminant in tap water for a hypothetical four-occupant household. That approach utilizes contaminant water-to-air transfer factors in conjunction with the model developed by Fisk et al. (1987) to estimate household-compartment concentrations of volatile contaminants in air. Therefore, the resulting exposure to TCE in indoor air was derived using Eq. 2.

$$E_{\text{Inh}} = \text{Inh} \times \frac{\left[\left(\frac{W_{\text{sh}} \times \phi_{\text{TCE-sh}}}{AE_{\text{sh}}} \times ET_{\text{sh}} \right) + \left(\frac{W_{\text{b}} \times \phi_{\text{TCE-b}}}{AE_{\text{b}}} \times ET_{\text{b}} \right) + \left(\frac{W_{\text{h}} \times \phi_{\text{TCE-h}}}{AE_{\text{h}}} \times ET_{\text{h}} \right) \right]}{D} \times ED \times \frac{EF}{AT} \times C_w, \quad (2)$$

where

- E_{inh} = TCE-exposure (intake) resulting from inhalation of TCE volatilized into indoor air from contaminated ground water used for domestic purposes [mg/(kg-d)];
- Inh = daily inhalation rate per unit body weight [$m^3/(kg-d)$];
- W_{sh} = water-useage rate per person for shower (L/h) [and also for bathroom, W_b (L/h)];
- W_h = water-useage rate for all household activities (L/h);
- ϕ_{TCE-sh} = water-to-air transfer efficiency of TCE in the shower (dimensionless);
- ϕ_{TCE-h} = water-to-air transfer efficiency of TCE in the house (dimensionless), and equal to $\phi_{TCE-sh} \times 0.54/0.70$ (where the fraction is the ratio of radon transfer in the shower to radon transfer in the house as reported by McKone and Bogen, 1992), with ϕ_{TCE-h} modeled as statistically independent of ϕ_{TCE-sh} ;
- AE_{sh} = air-exchange rate in the shower or bath stall (m^3/h);
- AE_b = air-exchange rate in the bathroom (m^3/h);
- AE_h = air-exchange rate in the house (m^3/h);
- ET_{sh} = exposure time in showering or bathing (h/d);
- ET_b = exposure time in bathroom (h/d);
- ET_h = exposure time in house (h/d);
- D = averaging time for daily water use (24 h/d);
- ED = exposure duration, also referred to as time of residence (y);
- EF = exposure frequency (d/y);
- AT = averaging time corresponding to a 70-y lifetime of exposure (d); and
- C_w = TCE concentration in ground water (mg/L).

Dermal uptake of TCE while showering or bathing is based on the model of Brown et al. (1984) and was calculated from the relationship shown in Eq. 3.

$$E_{Derm} = A \times f_s \times k_p \times ET_{sh} \times cf \times ED \times \frac{EF}{AT} \times \left[C_w \times \left(1 - \frac{\phi_{TCE-sh}}{2} \right) \right], \quad (3)$$

where

E_{Derm} = TCE-exposure (intake) resulting from dermal uptake of TCE while showering or bathing [mg/(kg-d)];

A = surface area of skin per unit body weight (cm²/kg);

f_s = fraction of total skin surface that is in contact with water during showering or bathing (dimensionless);

k_p = dermal permeability rate of TCE from dilute aqueous solutions (cm/h);

ET_{sh} = time spent showering or bathing (h/d);

cf = conversion factor (10⁻³ L/cm³)

ED = exposure duration, also referred to as time of residence (y);

EF = exposure frequency (d/y);

AT = averaging time corresponding to a 70-y lifetime of exposure (d); and

C_w = TCE concentration in ground water (mg/L);

$\phi_{\text{TCE-sh}}$ = water-to-air transfer efficiency of TCE in the shower (dimensionless);

Three concentration measurements of TCE were obtained in 1997 from a monitoring well at Site LF-13 on Beale Air Force Base (Purrier, 1997). This monitoring well is used for evaluating remediation efforts and is located in the immediate vicinity of the site of an extraction well that hypothetically could eventually supply ground water for domestic purposes to possible future residences in the surrounding area. Because soil-vapor extraction and air-stripping treatment of the ground water have been taking place at Site LF-13 to reduce the concentration of TCE to low-levels in the ground water (URSGWC, 1998), it is assumed that there are now no real differences between the three reported sample measurements and that the TCE concentration in the ground water is unlikely to be changing in time. On the basis of these assumptions (which are made for purposes of this illustration and require validation) and because there will be mixing and blending of the ground water during its extraction and

distribution, a hypothetical resident using such ground water domestically is likely to be exposed to the mean concentration. Accordingly, the uncertain mean TCE concentration in ground water was modeled as

$$C_w = \left[\frac{e^{\left(\tilde{\sigma}_{\log c_w} \right) \times T_2}}{E \left(e^{\left(\tilde{\sigma}_{\log c_w} \right) \times T_2} \right)} \right] \times \tilde{c}_w, \quad (4)$$

where

C_w = mean TCE concentration (mg/L), where uncertainty in $\log c_w$ is assumed to be T-distributed with two degrees of freedom;

$\langle C_w \rangle \equiv \tilde{c}_w$ = the sample mean of the three c_w measures (Purrier, 1997);

$\log c_w$ = sample mean of the three $\log c_w$ measures;

$\tilde{\sigma}_{\log c_w}$ = sample standard deviation of the three $\log c_w$ measures;

$\tilde{\sigma}_{\log c_w}$ = standard deviation of the sample mean of $\log c_w$, where

$$\tilde{\sigma}_{\log c_w} = \frac{\tilde{\sigma}_{\log c_w}}{\sqrt{3}} = 0.1295; \text{ and}$$

T_2 = variate distributed as Student's T with two degrees of freedom (see Appendix B for further explanation useful for constructing this distribution).

The expected-value term in Eq. 5, $E \left(e^{\left(\tilde{\sigma}_{\log c_w} \right) \times T_2} \right)$, was determined to be 1.0812, based on

a Monte-Carlo simulation involving 2000 trials. The bracketed term in Eq. 5 thus reflects a log- T_2 -distributed variate normalized to have an expected value equal to one.

Inter-household variability in water-to-air transfer efficiency of TCE in shower water ($\phi_{\text{TCE-sh}}$, which is a dimensionless term) was modeled based on 14 experimental

measures involving showers running water at ≥ 30 °C summarized by Corsi and Howard (1998). It was assumed that these measures reflect the effects on TCE transfer of variable conditions that may pertain to each household at risk over the course of any residential duration. Effective residential TCE water-to-air transfer efficiency, $\phi_{\text{TCE-sh}}$, was therefore estimated as the mean value of the reported measures (0.76), and variability in $\phi_{\text{TCE-sh}}$ was modeled by the relation

$$\phi_{\text{TCE-sh}} = 0.76 + \left(0.029 \times T_{\phi_{\text{TCE-sh}}} \right), \quad (5)$$

where 0.029 is the standard deviation of the mean of the measured values [which ranged from as much as 0.97 (for a 45 °C water temperature) to as low as 0.61 (for a 33 °C water temperature)], and $T_{\phi_{\text{TCE-sh}}}$ is a variate that has a Student's T distribution with 13 degrees of freedom (see Appendix B for further explanation useful for constructing this distribution).

The term $\left[C_w \times \left(1 - \frac{\phi_{\text{TCE-sh}}}{2} \right) \right]$ in Eq. 3 estimates the concentration of TCE in the water contacting the skin during showering, based on the assumption that TCE volatilization is approximately linearly proportional to the vertical distance water has fallen from the showerhead to the floor (Giardino et al., 1992), and that during showering the body contacts the water about half the distance between the showerhead and the floor. The term in Eq. 3 is also applicable to a bathing scenario, because approximately 30 to 47% of TCE volatilizes during bathtub-filling prior to bathing (see McKone, 1987).

Table 1 presents the input parameters identified or implied in Eqs. 1–3, but does not include the regulatory default values for such inputs, which appear in Table 2. In

Table 1, distributions for parameters are identified as representing either uncertainty or variability (heterogeneity) and corresponding distribution types are also listed. The exposure-model parameters treated as constants in this assessment are EF and AT . Other input variates were assumed to be distributed as summarized in Table 1 and as further described below. As indicated in Table 1, with the exception of the C_w and f_m variates, which are considered uncertain, all distributed input variates were assumed to be heterogeneous (i.e., to reflect interindividual variability).

The exposure duration (ED) term, in Eqs. 1–3 denotes household residence time in the area that would be supplied with the contaminated ground water for domestic purposes. Because ED should account for households moving into and out of the water-supply area, it is modeled to reflect nonlinear JUV. The procedure used to obtain \overline{ED} and $\langle ED \rangle$ distributions (and also a “rough,” but conservative, approximation of the 95th-percentile upper-bound value, \hat{ED} , of the cumulative probability distribution reflecting variability in exposure duration) adapts the Israeli and Nelson (1992) model of variability in the time of residence for households in the Western Region of the US. Specifically, this model defines the fraction $R(t)$ of households living in the same residence for a total of t years or more for the Western Region [see Eq. 12 and the corresponding parameter values in Table II of Israeli and Nelson (1992)].* According to this model,

$$l(s) = \frac{-d[\log R(s)]}{ds}, \quad (6)$$

* Note that we retain here the Israeli and Nelson (1992) notation for the fraction $R(t)$ as a function of time, which should not be confused with risk, R , defined (independent of time) in Eq. 13 of this report.

Table 1. Inputs (not including regulatory default values; see Table 2) for obtaining cancer risk-related estimators (see Table 3) for multiple-pathway exposure to low-levels of trichloroethylene (TCE) concentrations in ground water at Beale Air Force Base in California.

Variate (units)	Symbol	Distribution		Range		Arithmetic		Geometric		Percentile		Source of data
		Represents	Type ^a	Min.	Max.	Mean	Std. Dev.	Mean	Std. Dev.	5th	95th	
Mean TCE concentration in water (mg/L)	C_w	Uncertainty	log- T_2			0.0223					0.0301	Purrier (1997)
Fraction of emigrant residents moving out of a local water-supply district in western US (dimensionless)	f_m	Uncertainty	Tri	$\frac{1}{3}$	1	$\frac{2}{3}$	$\sqrt{\frac{1}{54}}$			0.439 ($=f_m^*$)		US Census Bureau (1997)
Cumulative distribution function for total residence time in the western US $\leq t$ (y)	$1-R(t)$	Variability	E			3.49						Israeli and Nelson (1992)
Approximate upper-bound residence duration (used to calculate \hat{R}_{High})	$\hat{ED} = \left[\frac{1 - R(t)^{f_m}}{f_m} \right]$	Variability	E								55.3	See Eqs. 8 and 11
Ingestion rate for western region of US [L/(kg-d)]	Ing	Variability	LN			0.0242	0.0170	0.0198	1.88		0.0399	Ershow and Cantor (1989) ^b

Table 1. (continued)

Variate (units)	Symbol	Distribution		Range		Arithmetic		Geometric		Percentile		Source of data
		Represents	Type ^a	Min.	Max.	Mean	Std. Dev.	Mean	Std. Dev.	5th	95th	
Inhalation rate [m ³ /(kg d)]	<i>Inh</i>	Variability	E			0.264				0.363		OEHHA (1996) and Marty (1998); and US Census Bureau (1998) ^b
Shower (and also bathroom) water-use rate(s) (L/h)	<i>W_{sh}</i> (and <i>W_b</i>)	Variability	LN			480	160	455	1.38	777		McKone and Bogen (1992), based on James and Knuiman (1987)
Household water-use rate (L/h)	<i>W_h</i>	Variability	LN			42.0	15.0	40.0	1.41	69.9		McKone and Bogen (1992), based on James and Knuiman (1987)
Normalized mean water-to-air transfer efficiency for TCE (dimensionless)	<i>T_{φ_{TCE-sh}}</i>	Variability	<i>T₁₃</i>			0				1.771		Corsi and Howard (1998)
Air-exchange rate for shower (m ³ /h)	<i>AE_{sh}</i>	Variability	U	4.0	20.0	9.94 ^c				4.82 ^c		McKone and Bogen (1992)

Table 1. (continued)

Variate (units)	Symbol	Distribution		Range		Arithmetic		Geometric		Percentile		Source of data
		Represents	Type ^a	Min.	Max.	Mean	Std. Dev.	Mean	Std. Dev.	5th	95th	
Air-exchange rate for bathroom (m ³ /h)	AE_b	Variability	U	10.0	100.0	39.1 ^c				14.6 ^c		McKone and Bogen (1992)
Air-exchange rate for house (m ³ /h)	AE_h	Variability	U	300	1200	649 ^c				344 ^c		McKone and Bogen (1992)
Exposure time in shower (h/d)	ET_{sh}	Variability	LN			0.129	0.052	0.120	1.47		0.226	Burmaster (1998)
Exposure time in bathroom (h/d)	ET_b	Variability	LN			0.330	0.220	0.274	1.83		0.744	McKone and Bogen (1992)
Exposure time in house (h/d)	ET_h	Variability	U	8.0	20.0	14.0					19.4	McKone and Bogen (1992)
Surface area per unit body weight (cm ² /kg)	A	Variability	E			326					373	Phillips et al. (1993); and US Census Bureau (1998) ^b
Fraction of skin exposed in shower or bath (dimensionless)	f_s	Variability	U	0.40	0.90	0.65					0.875	McKone and Bogen (1992)
Skin-permeability coefficient (cm/h)	k_p	Variability	N			0.263	0.018				0.293	Bogen et al. (1998)

Table 1. (continued)

Variate (units)	Symbol	Distribution		Range		Arithmetic		Geometric		Percentile		Source of data
		Represents	Type ^a	Min.	Max.	Mean	Std. Dev.	Mean	Std. Dev.	5th	95th	
Cancer slope factor applicable to both ingestion and dermal exposures {R/[mg/(kg-d)]}	CSF_{Ing} (and also CSF_{Derm})	Not applicable	C								0.015	CalEPA (1996)
Cancer slope factor applicable to inhalation exposure {R/[mg/(kg-d)]}	CSF_{Inh}	Not applicable	C								0.010	CalEPA (1996)
Averaging time for 70-y lifespan (d)	AT	Not applicable	C		25,550							USEPA Region 9 (1998) and USEPA (1989)
Exposure frequency (upper-bound value; d/y)	EF	Not applicable	C		350							USEPA Region 9 (1998) and USEPA (1991)

^a Distribution types: C = constant; E = empirical (or fitted); LN = lognormal; N = normal; T_{df} = Student's T with df equal to degrees of freedom; log- T_{df} = exponentiated T_{df} distribution; Tri = triangular, U = uniform.

^b Upper-bound (95th percentile) values for lifetime, time-weighted-average quantities calculated using information from the cited references (see Methods).

^c Mean and corresponding 5-percentile values associated with each air-exchange (AE) rates were obtained from the inverse-uniform distribution (1/U) that was constructed from a Monte-Carlo simulation, involving 2,000 trials, of the uniform distribution. Thus, values reported in units of the data are the harmonic mean and the inverse of the 95th percentile of 1/U. This was done so that expected values of risk-related estimators could be calculated using the corresponding exact expressions (which include AE values appearing as denominators—see Eq. 2).

Table 2. Inputs and corresponding regulatory default values applicable to a deterministic calculation of excess-lifetime cancer risk for a “reasonably maximum exposed” person (\hat{R}_{RME}).^a

Variate (units)	Value	Reference
Ingestion rate (L/d)	2.0	USEPA Region 9 (1998); USEPA (1989)
Body weight (kg)	70.0	USEPA Region 9 (1998); USEPA (1989)
Inhalation rate (m ³ /d)	20.0	USEPA Region 9 (1998); USEPA (1989)
Exposure time in house (h/d)	16.4	USEPA Region 9 (1998); Tsang and Klepeis (1996)
Shower duration (h/d)	0.13	USEPA (1997); James and Knuiman (1987)
Skin-surface area (cm ²)	23,000.0	CalEPA/DTSC (1994)
Residential-exposure duration (y)	30.0	USEPA Region 9 (1998); USEPA (1989)
Residential-exposure frequency (y)	350.0	USEPA Region 9 (1998); USEPA (1991)
Averaging time (d)	25,550.0	USEPA Region 9 (1998); USEPA (1989)
Ingestion (and used for dermal) cancer-slope factor (CSF_{Ing}) {Risk/[mg/(kg d)]}	0.015	CalEPA (1996)
Inhalation cancer-slope factor (CSF_{Inh}) {Risk/[mg/(kg d)]}	0.01	CalEPA (1996)

^a Characterizing risk for the “reasonable maximum exposure” case involves combining upper-bound and mid-range factors so that a conservative estimate (i.e., above the average) results that is within the range of reasonable possibilities, and is not the worst-possible case (USEPA, 1989 and 1991). The inputs to the \hat{R}_{RME} identified here are consistent with this goal. Specifically, the inputs and corresponding regulatory default values shown are used. Where default values are not given (and cannot be obtained from those shown) for *uncertain* variates (e.g., TCE concentration in water) the expected value for that input is used (see Table 1). Similarly, in the absence of default values for *heterogeneous* variates (e.g., water-use rates) the 95%-tile value for that input is used (see Table 1); unless the heterogeneous variate was in the denominator of an equation (e.g., air-exchange rates), and then the 5%-tile value is used (see Table 1 and also footnote c of Table 1).

where $0 \leq s \leq t$ and $l(s)$ is the rate of household moves, implying that $R(t)$ is modeled as a single “compartment” with loss rate $l(s)$ for $0 \leq s \leq t$, i.e., as

$$R(t) = R_0 e^{-\int_0^t l(s) ds}, \quad (7)$$

where $R_0 = R(0) = 1$, and $R(\infty) = 0$. Now, let f_m be the fraction of household moves that are “effective”, because they involve moves out of an area of concern (in our case, a hypothetical future water-supply district). Thus,

$$R_{f_m}(t) = e^{-\int_0^t l(s) \times f_m ds} = [R(t)]^{f_m}, \quad (8)$$

where $R(t)$ is heterogeneous and f_m is uncertain. Based on geographic mobility data reported by the US Census Bureau (1997), about $\frac{2}{3}$ of all US moves are within the same county. We assume that these moves include an uncertain fraction $(1 - f_m)$ that are within the same water-supply district, and that $(1 - f_m)$ is triangularly distributed between 0 and $\frac{2}{3}$ with a mode at $\frac{1}{3}$, which is consistent with data indicating that many households move small distances within corresponding local areas (ARC, 1999; and Duke-Williams, 1999). Thus, as indicated in Table 1 we assume f_m is triangularly distributed between $\frac{1}{3}$ and 1 with a mode at $\frac{2}{3}$.

The population-average value of total residence time, \overline{ED} , with respect to variability in ED , is defined by Israeli and Nelson (1992) as

$$\overline{ED} = \int_0^\infty R(t) dt, \quad (9)$$

(i.e., conditional on $f_m = 1$). It follows that for any value of f_m , the corresponding population-average value of uncertain total residence time is specified by

$$\overline{ED} = \int_0^\infty R_{f_m}(t) dt = \int_0^\infty [R(t)]^{f_m} dt, \quad (10)$$

in which uncertainty in f_m was discussed above.

The cumulative probability distribution reflecting variability in total time of residence, t , is defined as $1 - R(t)$, in the model of Israeli and Nelson (1992; see their Eq. 4). The corresponding definition of variability in expected ED , conditional on f_m , is given by

$$\langle ED \rangle = 1 - R_{f_m}(t), \quad (11)$$

which, in view of the nonlinear relationship between uncertainty and heterogeneity in $R_{f_m}(t)$, was approximated using a second-order estimate of $\langle R_{f_m}(t) \rangle$ (see Bogen and Spear, 1987):

$$\begin{aligned} \langle ED \rangle &= 1 - R_{f_m}(t) = \langle 1 - [R(t)]^{f_m} \rangle \\ &\approx 1 - \left\{ [R(t)]^{f_m} + \left(\frac{1}{2} \times \frac{\partial^2 R_{f_m}(t)}{\partial f_m^2} \times \sigma_{f_m}^2 \right) \right\} \\ &\approx 1 - \left\{ [R(t)]^{f_m} \times \left(1 + \frac{\{\ln[R(t)]\}^2 \times \sigma_{f_m}^2}{2} \right) \right\}, \end{aligned} \quad (12)$$

the final step of which follows from the fact that $\frac{\partial^2 x^a}{\partial a^2} = x^a [\ln(x)]^2$ for any x independent of a .

Further details concerning procedures useful for obtaining \hat{ED} , and \overline{ED} and $\langle ED \rangle$ distributions are presented in Appendix B.

Cancer-Risk Model

Because hypothetical residential low-dose exposure to TCE, such as might occur as a result of groundwater contamination at Site LF-13 of Beale Air Force Base, is assumed to have a positive, nearly constant slope at doses small enough to ensure lifetime excess cancer risk, R , is substantially less than one (i.e., $R \ll 1$), R can be estimated by Eq. 13:

$$R \cong (E_{\text{Ing}} \times CSF_{\text{Ing}}) + (E_{\text{Derm}} \times CSF_{\text{Ing}}) + (E_{\text{Inh}} \times CSF_{\text{Inh}}), \quad (13)$$

where CSF_{Ing} is the oral cancer slope factor (CSF) for TCE [assumed to apply to both ingestion and dermal exposures (CalEPA/DTSC, 1994; USEPA Region 9, 1998)], and CSF_{Inh} is the inhalation CSF for TCE that are reported by CalEPA (1996). Each CSF represents an upper-bound estimate of the probability of cancer per unit intake of TCE and unit body weight over a lifetime $\left[\text{i.e., } \frac{\text{Risk}}{\text{mg}/(\text{kg} \cdot \text{d})} \right]$. The CSF_{Ing} and CSF_{Inh} parameters are treated as constants (Table 1).

The more traditional approach for arriving at estimators of risk can involve substituting into Eq. 13 those values for E_{Ing} , E_{Inh} , and E_{Derm} that were all obtained using input parameters either at (1) means only, (2) regulatory defaults, in combination with mean values for parameters that are uncertain and upper bounds (e.g., 95th percentiles, or where applicable 5th percentiles, see footnote c in Table 1) for parameters that are heterogeneous, where default values for such variates are not available or (3) upper bounds exclusively (e.g., 95th percentiles, or where applicable 5th percentiles, see footnote c in Table 1). In the first case, the value of R equates to a “best” estimate, \hat{R}_E . In the second case, the value of R is considered to be for a “reasonably maximum exposed” person, \hat{R}_{RME} . In the third case, the value of R corresponds to an upper

“conservative” bound, \hat{R}_{High} . All three of these types of risk-related estimators were calculated so these traditional-type estimators could be compared to analogous risk estimators that are more explicitly defined regarding uncertainty and/or variability. The input means used for calculating \hat{R}_E and the input upper bounds [e.g., 95th percentiles; or where applicable, the 5th-percentile values (see footnote c in Table 1)] used for calculating \hat{R}_{High} all appear in Table 1. The default inputs used for calculating \hat{R}_{RME} appear in Table 2, with the expected values and 95th-percentile upper-bound values [or where applicable, 5th-percentile values (see footnote c in Table 1)] appearing in Table 1 for those uncertain and heterogeneous variates, respectively, for which default values are not given. Thus, the \hat{R}_{RME} is considered to be a conservative estimate of risk (i.e., above the average) that is within the range of reasonable possibilities, and is not the worst-possible case (USEPA, 1989 and 1991).

Risk-related estimators explicitly defined regarding uncertainty and/or variability involve the conditional expectations \bar{R} and $\langle R \rangle$ (Bogen and Spear, 1987; NRC, 1994; Bogen, 1995). \bar{R} -type estimators of risk involve \bar{R} , which represents uncertain lifetime cancer risk to a (hypothetical) person at a population-average level of risk relative to others. The symbols $\bar{R}_{.05}$ and $\bar{R}_{.95}$ are used to represent the two-tailed lower and upper 90% confidence limits on the cumulative distribution function (cdf) of \bar{R} ; and $\langle \bar{R} \rangle$ denotes the expected value (i.e., expectation with respect to uncertainty) of \bar{R} . $\langle R \rangle$ -type estimators of risk involve $\langle R \rangle$, which denotes the set of expected values (with respect to uncertainty) of all the (potentially) different (“heterogeneous”) cancer risks incurred within the population at risk. Thus, $\langle R \rangle_{.05}$ and $\langle R \rangle_{.95}$ represent the two-tailed lower and upper 90% confidence limits on the cdf $\langle R \rangle$; and $\langle \bar{R} \rangle$ is the

population-average value of $\langle R \rangle$. (Note that the “population average” or arithmetic-mean value of a heterogeneous variate is just the expected value of that variate within a defined population. Expectations of lifetime-excess cancer risk, R , with respect to variability (i.e., \bar{R}) and uncertainty (i.e., $\langle R \rangle$) are defined by

$$\bar{R} = (\bar{E}_{\text{Ing}} \times CSF_{\text{Ing}}) + (\bar{E}_{\text{Inh}} \times CSF_{\text{Inh}}) + (\bar{E}_{\text{Derm}} \times CSF_{\text{Ing}}), \text{ and} \quad (14)$$

$$\langle R \rangle = (\langle E_{\text{Ing}} \rangle \times CSF_{\text{Ing}}) + (\langle E_{\text{Inh}} \rangle \times CSF_{\text{Inh}}) + (\langle E_{\text{Derm}} \rangle \times CSF_{\text{Ing}}), \quad (15)$$

where the terms E_{Ing} , E_{Inh} , and E_{Derm} are defined in Equations 1–3, and CSF_{Ing} and CSF_{Inh} are described in the text following Eq. 13 (i.e., treated as constants and reported by CalEPA/DTSC, 1994; and/or USEPA Region 9, 1998).

The term R^* denotes an upper-bound estimate with respect to JUV in risk. Specifically, $R_{.95}^*$ denotes the risk to an individual who is at a 95th-percentile level of risk relative to those risks incurred by others in the population at risk. Alternative first-order approximations of this upper-bound JUV estimator (see Bogen, 1995) are given by

$$R_{.95}^* = \bar{R}_{.95} \times \rho_{.95} \quad \text{or} \quad R_{.95}^* = \langle R \rangle_{.95} \times \rho'_{.95}, \quad (16)$$

where the terms $\rho_{.95}$ and $\rho'_{.95}$ denote “dispersion” ratios between upper-bound risk and expected individual risk; that is,

$$\rho_{.95} = \frac{\langle R \rangle_{.95}}{\langle R \rangle} \quad \text{and} \quad \rho'_{.95} = \frac{\bar{R}_{.95}}{\langle \bar{R} \rangle}. \quad (17)$$

Note that $\rho_{.95}$ may be interpreted as an index of the “inequity” reflected in the distribution of individual risks incurred by a population at risk, insofar as this ratio is proportional to the variance (which measures interindividual differences) in that population. Similarly, $\rho'_{.95}$ represents an index of uncertainty associated with individual risk.

For a population of size n_T , N is used to denote the uncertain number of additional cancer cases due to R , where expected number of cases is defined as $\langle N \rangle = n_T \times \langle \bar{R} \rangle$. Of specific interest to stakeholders and decision makers may be the probability, $1 - P_0$, that for a given population n_T , there will be one or more additional cases of cancer (i.e., the probability that $N \geq 1$).

The value of P_0 can be well approximated generally (see Bogen and Spear, 1987; NRC, 1994; Bogen, 1995) by the integral of the conditional Poisson likelihood function:

$$P_0 \approx \int_0^1 e^{-n_T \bar{R}} f_{\bar{R}}(\bar{R}) d\bar{R} , \quad (18)$$

where the compound-Poisson variate, $n_T \bar{R}$, incorporates the uncertain parameter \bar{R} defined in Eq. 14. (Further details concerning the procedure for obtaining P_0 can be found in the last section of Appendix B.)

Calculations

Variabilities in route-specific intake-related quantities (Ing , Inh , A —defined after Eqs. 1, 2, and 3, respectively) were calculated using corresponding demographic and exposure-related data cited in Table 1. Note that variability in each quantity necessarily depends on the duration of exposure (ED) experienced by the population at risk. If all

people were exposed for an entire lifetime, then this variability is properly characterized as the distribution of the lifetime, time-weighted-average (TWA) value of the corresponding quantity (*Ing*, *Inh*, or *A*). In contrast, if exposure duration were in all cases very brief, then this variability for each quantity would better be characterized as the composite distribution reflecting the weighted (or “age-adjusted”) average of the age-specific distributions of that quantity, using age-specific population fractions as weights.

For the present analysis, all calculations of \hat{R}_{High} used upper-bound (95th percentile) values (listed in Table 1) of the lifetime TWA distributions of variability in *Inh*, *Ing*, and *A* (\hat{R}_E and \hat{R}_{RME} used means listed in Table 1 and default values listed in Table 2, respectively, for these same three inputs). All other output risk-characterization quantities were calculated using corresponding composite, “age-adjusted” distributions reflecting people of all ages within the modeled exposed population. The latter procedure used is necessarily “conservative”, in the sense that for each quantity the composite distribution (which is a weighted mixture of age-specific distributions) is necessarily more broad (i.e., has a larger variance) than the corresponding lifetime TWA distribution (which is the distribution of a weighted sum of random variate values). Thus, the larger *ED*, the more likely exposure will involve more than one of the age ranges used to construct the composite distribution, and hence the relevant quantity would more accurately be calculated as a TWA value involving the age ranges involved.

Ideally, computation would involve sampling a value of *ED* as well as a starting age, and then calculating (or, via a lookup method employing pre-calculated distributions, selecting) the relevant variability distributions for *Ing*, *Inh*, and *A*. This procedure is numerically taxing, however, so the alternative, simpler, albeit somewhat

conservative, approach described above was used instead. This approach implies only very little conservatism in the case of risk characterizations involving $\langle R \rangle$, because the $\langle ED \rangle$ distribution was highly skewed (with a median value of only approximately 2 y), due to the highly skewed nature of residential turnover $R(t)$. Somewhat greater conservatism is implied for risk characterizations involving \bar{R} , because \overline{ED} , not nearly as skewed, has a median value of approximately 7 y.

For the reasons discussed above, the calculation of E_{Ing} was based on the Ershow and Cantor (1989) lognormal approximation of the composite distribution reflecting variability in tap-water ingestion per kg body weight by people of all ages in the Western Region of the US. The corresponding lifetime TWA distribution was calculated assuming a 70-y lifespan and using the age-specific intakes reported by Ershow and Cantor (1989). The mean for both distributions was nearly the same.

The calculation of E_{Inh} was based on age-specific rates of total inhalation per kg body weight for California youth and adults (data collected by Adams, 1993, and Wiley et al., 1991a,b; were reevaluated and presented by OEHHA, 1996; according to discussion with Marty, 1998). From these data a corresponding composite distribution was calculated using youth and adult population weights derived from national census data (USCB, 1998), and a corresponding lifetime TWA distribution was calculated using $\frac{12}{70}$ and $\frac{58}{70}$ as exposure-duration weights for youth and adults, respectively. The mean for both distributions was the same.

The calculation of E_{Derm} was based on age-specific estimates of body surface area per kg body weight, A , reported by Phillips et al. (1993). From these data a corresponding composite distribution was calculated using infant/toddler, youth, and adult population weights derived from national census data (USCB, 1998), and a

corresponding lifetime TWA distribution was calculated using $\frac{2}{70}$, $\frac{16}{70}$, and $\frac{52}{70}$ as exposure-duration weights for the respective age groups. The mean for both distributions was the same.

Calculations of derived input-variate distributions, the output \bar{R} and $\langle R \rangle$ distributions, and related estimators were performed by Monte-Carol simulations using *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996), and/or *Mathematica*®, version 3.0 (Wolfram, 1996). Appendix B contains further explanations of (1) additional procedures useful for generating several different input-variate distributions and corresponding expected values and upper bounds; (2) the approach for deterministically calculating exposure and traditional risk-related (point) estimators; and (3) methods for estimating the probability of zero additional cases of cancer (P_0).

RESULTS

Table 3 summarizes the lifetime excess cancer risk-related estimates for hypothetical residents theoretically supplied ground water from beneath Site LF-13 at Beale Air Force Base that contains the 1997 measured, low-level concentrations of TCE (Purrier, 1997). The traditional risk-related estimator approach yields values of \hat{R}_E , \hat{R}_{RME} , and \hat{R}_{High} equal to 3.1×10^{-6} , 6.1×10^{-5} , and 2.4×10^{-4} , respectively [further details concerning the calculations of these traditional risk-related (point) estimators and also those for exposure (i.e., daily dose or intake) can be found in Table B-4 and related text of Appendix B]. The risk-related estimator approach that is explicit regarding

Table 3. Lifetime excess cancer risk-related estimates for hypothetical residents adjacent to Beale Air Force Base in California, based on multiple-pathway (i.e., ingestion, inhalation, and dermal) exposures to ground water containing low-levels of trichloroethylene (TCE).

Risk-related estimator approach ^a Type of estimator	Symbol ^a	Value	CVM (%) ^b
Traditional			
"Best" estimate (using input means)	\hat{R}_E	3.1×10^{-6}	NA
Risk to "reasonably maximum exposed" person	\hat{R}_{RME}	6.1×10^{-5}	NA
Upper "conservative" bound	\hat{R}_{High}	2.4×10^{-4}	NA
Explicit regarding uncertainty and/or variability in:			
> population-average risk, \bar{R}			
Expectation (with respect to uncertainty)	$\langle \bar{R} \rangle$	3.1×10^{-6}	NA
Lower uncertainty bound	$\bar{R}_{.05}$	1.4×10^{-6}	0.46
Upper uncertainty bound	$\bar{R}_{.95}$	5.5×10^{-6}	0.45
> expected risk (with respect to uncertainty), $\langle R \rangle$			
Population average	$\overline{\langle R \rangle}$	3.1×10^{-6}	NA
Lower variability bound	$\langle R \rangle_{.05}$	3.6×10^{-8}	0.97
Upper variability bound	$\langle R \rangle_{.95}$	1.4×10^{-5}	1.2
> jointly uncertain and heterogeneous risk			
Index of "inequity" in expected risk	$\rho_{.95}$	4.7	0.58
Upper JUV bound	$R_{.95}^*$	2.6×10^{-5}	0.62

^a Note that \hat{R}_E , $\langle \bar{R} \rangle$, and $\overline{\langle R \rangle}$ denote three closely related estimators of mean risk; that \hat{R}_{RME} and \hat{R}_{High} are crude and typically conservative approximations of $R_{.95}^*$; and that JUV refers to joint uncertainty and variability.

^b Coefficient of variation of the mean (expressed in percent), $CVM\% = 100\% \times \frac{\tilde{\sigma}}{\bar{X} \times \sqrt{m}}$,

where $\tilde{\sigma}$ is the sample standard deviation and \bar{X} is, for each estimator, the sample arithmetic mean obtained from m equal to 10 repeated Monte-Carlo simulations each involving 2,000 trials. Small CVM% values (i.e., < 2%) indicate the estimates obtained are highly reliable, despite Monte-Carlo sampling error. A CVM% value is not applicable (NA), when value of risk-related estimator was not estimated by simulation, but rather was calculated using the corresponding exact expression.

uncertainty in population-average risk, \bar{R} , produces a value for $\langle \bar{R} \rangle$ equal to 3.1×10^{-6} , and two-tailed lower and upper 90% confidence limits on the cdf of \bar{R} equal to 1.4×10^{-6} for $\bar{R}_{.05}$, and 5.5×10^{-6} for $\bar{R}_{.95}$. The risk-related estimator approach that is explicit regarding variability in expected risk (with respect to uncertainty), $\langle R \rangle$, produces a value for $\langle \bar{R} \rangle$ equal to 3.1×10^{-6} , and two-tailed lower and upper 90% confidence limits on the cdf of $\langle R \rangle$ equal to 3.6×10^{-8} for $\langle R \rangle_{.05}$ and 1.4×10^{-5} for $\langle R \rangle_{.95}$. The index of “inequity” in expected risk (or “dispersion” ratio), $\rho_{.95}$, equals 4.7, which is not substantial (i.e., less than a factor of 10) and therefore indicates there is not a great amount of interindividual variability within the population in this situation. The upper JUV bound ($R_{.95}^*$), which is approximated by the product of $\bar{R}_{.95}$ and $\rho_{.95}$ equals 2.6×10^{-5} . (The result was nearly identical using $\rho'_{.95}$ to estimate $R_{.95}^*$ —see Eq. 16). Both the upper-bound population-average risk estimator, $\bar{R}_{.95}$, and the upper-JUV-bound risk estimator, $R_{.95}^*$, have values less than 10^{-4} and within the range of acceptability (i.e., 10^{-4} to $\leq 10^{-6}$) with respect to generally followed regulatory guidance (USEPA, 1990).

Table 4 contains the results of the analysis of population risk associated with multipathway exposures to the TCE-contaminated ground water. These results reveal that the probability ($1 - P_0$) of greater than zero additional cases of cancer for local on-ground, exposed populations of up to several hundred (i.e., corresponding to n individuals; which is the reasonably foreseeable short-term scenario), is less than 0.01. Even for n up to 26,900, the probability of more than zero cases remains below 0.5.

Table 4. Population risk associated with multipathway exposures to TCE-contaminated ground water at Beale Air Force Base in California.

Total exposed population over 70 y, n_T	Exposed population during 7.6 y, n^a	Probability of > 0 additional cases of cancer, $1 - P_0^b$	CVM ^c	Expected value of the total number of additional cancer cases, $\langle N \rangle = n_T \times \langle \bar{R} \rangle$
100	11	0.0003	0.00030%	0.00031
2,000	217	0.0063	0.0053%	0.0062
30,000	3,257	0.0879	0.022%	0.094
247,766.9	26,900	0.5000	0.031%	0.77

^a Here n denotes the number of individuals residing at the impacted site within any 7.6-y time interval (i.e., the expected value, $\langle \overline{ED} \rangle$, of uncertain exposure duration, \overline{ED} , for the average exposed person) during the total 70-y time period considered (i.e., $n = n_T \times \frac{7.6 \text{ y}}{70 \text{ y}}$). Note that n is not used to compute P_0 , and is shown rounded to the nearest integer.

^b Each value listed is the mean of 10 estimates obtained using the \bar{R} distributions generated by 10 corresponding Monte-Carlo simulations, each involving 2,000 trials (see Appendix B for further explanation).

^c Coefficient of variation of the mean (CVM, and expressed in percent) was derived as explained in Table 3, footnote b.

In fact, the expected value of the total number of additional cancer cases remains less than 0.01 for n up to several hundred and does not exceed 0.5 until n exceeds 26,900. Even then, it is not clear that the extraction well would be capable of supporting such a large on-ground population, or even the comparable total exposed population over 70 y (i.e., n_T) that is equal to 247,767.

The Monte-Carlo sampling errors indicated in Tables 3 and 4 are all small [i.e., coefficient of variation of the mean (CVM), expressed in percent (%) < 2%; see

footnote b in Table 3 for equation]. This result addresses the issue of Monte-Carlo quality-control and assures that corresponding estimates are highly reliable.

DISCUSSION AND CONCLUSIONS

Bogen (1995) has shown that upper-bound estimators of JUV in risk may be approximated using calculations involving cumulative distribution functions (cdfs) that reflect only uncertainty and only interindividual variability, thus avoiding relatively tedious "nested" Monte-Carlo techniques that are otherwise required to obtain estimators of JUV in risk. The approximation procedure was successfully employed for this analysis of uncertainty and variability in exposure to characterize risk from TCE-contaminated ground water at Site LF-13 on Beale Air Force Base in California. Comparing the results of this approach to the more traditional one shows that the risk-estimators computed more traditionally overestimate the risk to an upper-bound individual R_{95}^* , when JUV in the population is addressed explicitly. Furthermore, it can be seen from the results in Table 3 that \hat{R}_E , $\langle \bar{R} \rangle$, and $\overline{\langle R \rangle}$ all represent expected risk to the average individual. The equality between $\langle \bar{R} \rangle$ and $\overline{\langle R \rangle}$ (and hence the consistency between the alternative R_{95}^* estimates) suggests that the first-order approximation approach for R_{95}^* is reliable in this case. More accurate R_{95}^* estimation would require numerically intensive nested Monte-Carlo methods.

Results presented in Table 4 indicate that the greater the exposed population, the less likely will be the chance that there will be zero observed cases. However in this analysis, for n in the hundreds, there is a probability of less than 0.01 that the number of additional cases will be greater than zero. Even for n up to 26,900, the probability of

more than zero cases remains less than 0.5. Clearly, this information is more valuable than that provided by a single, point estimate of $\langle N \rangle$ alone, especially for large populations (e.g., n_T is 247,767) where $\langle N \rangle$ approaches but does not exceed 1, and there is really no measure of confidence (or uncertainty) associated with just that expected value.

On the basis of this risk analysis of the TCE-contaminated ground water beneath Site LF-13 at Beale Air Force Base, and as pointed out by Bogen (1995), specific risk estimators might provide the bases for risk-acceptability criteria for a site, along with a specified value for $1 - P_0$. For example, risk-acceptability criteria might take the form of a joint requirement that \bar{R}_{95} be at least within range of generally followed regulatory guidance 10^{-6} to 10^{-4} (USEPA, 1990); and $\rho_{95} < 10^2$; $R_{95}^* \leq 10^{-4}$; and $1 - P_0 < 0.5$. Under such conditions, the upper-bound population-average risk, \bar{R}_{95} , is low and within generally accepted regulatory limits; there does not appear to be a great amount of interindividual variability within the population, because the index of "inequity" in expected risk, ρ_{95} is not substantial and so special susceptible groups do not need consideration; relatively highly exposed people in the population are not incurring inordinate risk as R_{95}^* is even less than 10^{-4} ; and the probability of 1 or more cases of cancer is less than 0.5 for a reasonably foreseeable population equal to n and an expected exposure duration of 7.6 y. Clearly, the results presented here for the TCE-contamination of ground water addressed at Site LF-13 at Beale Air Force Base meet these requirements and such risk criteria for this site can ensure that individual lifetime risks are both *de minimis* and equitable.

The more traditional estimates of risk in this case all overestimate the level of risk to the upper-bound individual, including \hat{R}_{RME} . Therefore, while providing an

expedient and standardized assessment tool for screening risk levels at a particular site, such traditional approaches to estimating risk will always overestimate upper-bound individual risk, and may lead regulatory agencies to impose more stringent and costly remediation standards than might otherwise be appropriate. The approach illustrated in this report for TCE-contaminated ground water at Site LF-13 on Beale Air Force Base demonstrates a systematic mechanism for deriving risk-acceptability criteria that can help convince decision makers and stakeholders that money and resources being dedicated to remediation might better spent on other public health measures that might be more cost effective.

The results of this work reinforce the importance of considering variability and uncertainty in estimates of risk. They also illustrate that the calculations can be readily performed by applying commercially available software for desktop computers, and will yield information of sufficient detail to establish reasonable and equitable site-specific risk-acceptability criteria.

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APPENDIX A

Glossary of Important Terms

Terminology	Explanation
Constant	An input parameter that is assumed to be correct—neither uncertain nor variable.
Deterministic, screening-level calculation of exposure and risk	A model that commonly involves using upper-bound point estimates for input parameters that are not considered to be constant in order to generate a conservative point estimate of risk.
Exposure pathways considered	Direct ingestion (E_{ing}) of substance-contaminated groundwater; inhalation (E_{inh}) of substance volatilized from contaminated groundwater into residential indoor air; and dermal absorption (E_{derm}) of substance while using contaminated groundwater for showering or bathing [contaminant intake from each exposure pathway is expressed in units of mg/(kg-d); see Eqs. 1, 2, and 3, respectively].
Interindividual variability	True differences (i.e., heterogeneity) in a risk-related characteristic (e.g., physiological differences) associated with different individuals in a population at risk (see Table 1).
Joint uncertainty and interindividual variability (JUV) in predicted risk	The uncertainty and interindividual variability in predicted risk, based on the uncertainty and/or interindividual variability in one or more input parameters.
JUV notation: overbar and angle brackets	An overbar (i.e., $\overline{}$) denotes mathematical expectation with respect to heterogeneous parameters only, and angle brackets (i.e., $\langle \rangle$) denote mathematical expectation with respect to uncertain parameters only. Additionally, $\langle \overline{} \rangle$ represents expectation with respect to uncertainty, after expectation with respect to heterogeneity, and $\overline{\langle \rangle}$ represents a population-average value of expectations with respect to uncertainty.

Glossary of Important Terms (continued)

Terminology	Explanation
Monte-Carlo simulation	A mechanism for randomly selecting values from an input distribution or distributions in order to generate an output distribution for a probabilistic model.
Probabilistic approach to estimating exposure and risk	A model that permits the entire distribution of an input parameter, which is not considered to be constant, to be used and combined with distributions of other input parameters, as well as constants, in order to generate a distribution for possible outcomes.
Total Risk (<i>R</i>)	The increased lifetime probability of cancer for an individual attributable to exposure to a chemical by one or more physiological intake pathways (e.g., ingestion, inhalation, and dermal absorption) (see Eqs. 13 through 15 in text).
Uncertainty	Lack of knowledge concerning the true value of a risk-related variate (see Table 1 in text).

APPENDIX B

Further Explanations of

(1) Additional Procedures Useful for Generating Several Different Input-Variate Distributions, and Corresponding Expected Values and Upper-Bounds; (2) The Approach For Deterministically Calculating Exposure and Traditional Risk-Related (Point) Estimators, and (3) Methods for Estimating the Probability of Zero Additional Cases of Cancer (P_0)

In order to address uncertainty and variability in exposure (as noted in Eq. 14 and 15 in text), as well as obtain more traditional values equating to a “best” estimate, a “reasonable maximum exposure”, and an upper “conservative” bound for exposure and risk, appropriate distributions for input variates must be constructed and used for nonconstant terms in Eqs. 1 through 3 in text (also see Table 1 in text). For example, details of distribution types and attributes for all inputs of water-use rates and water-exposure times (see Eq. 2 in text), as well as for the skin-permeability coefficient (see Eq. 3 in text), were obtained directly from the literature (see Table 1 in text). One purpose of this appendix is to provide further explanation of additional methods involving a combination of a spreadsheet and *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) computer software that can be used to construct several of the other input-variate distributions used by Eqs. 1 through 3, respectively, in text. Another purpose is to present the details of the approach for calculating traditional exposure and traditional risk-related (point) estimators. Finally, this appendix describes the procedure that can be performed using a spreadsheet and *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) computer software to estimate the probability of zero additional cases of cancer P_0 [and its complement, the probability of one or more (i.e., > 0) additional cases of cancer, $1 - P_0$] in a total population, n_T , over a 70-year period. The explanations provided assume that the reader is familiar with the purpose and use of commercially

available spreadsheet computer software and also software for performing Monte-Carlo simulations [e.g., *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996)].

Exposure-Pathway Specific Intakes

As discussed in the “Calculations” section of the text, two types of cumulative distribution functions (cdfs) for each of the three route-specific intake-related quantities (i.e., *Ing*, *Inh*, and *A*—defined after Eqs. 1, 2, and 3, respectively, in text) need to be derived. The first type of cdf is a composite distribution reflecting the weighted functional average of age-specific cdfs for that quantity, using age-specific population fractions as weights. The composite distribution applies to someone picked at random from the population having an exposure duration likely to be experienced by the population at risk. The second type of cdf is a lifetime, time-weighted-average (TWA) distribution that represents a stochastic weighted sum of independent variate values each sampled from a corresponding age-specific cdf, using the corresponding fraction of lifespan as the weight. The expected (mean) and upper-bound (95th-percentile) values obtained from the lifetime, TWA distribution are used when considering characterizing exposure and risk for a person exposed for their entire lifetime.

Ingestion rate of drinking water [Ing; L/(kg-d)]

Ershow and Cantor (1989) derive a composite distribution reflecting variability in the ratio (*Ing*) of tap-water ingestion rate to body weight [L/(kg-d)] for people of both sexes in age groups between 0 y and over 65 y during all seasons in the Western Region of the US (see bottom row of Table B-1 for moments of composite distribution). This composite distribution is

Table B-1. Weighting factor and age-specific ratios (*Ings*) of tapwater intakes to body weights [L/(kg-d)] for both sexes and all seasons for Western Region of US [from Table 36 in Ershow and Cantor (1989)].

Age (y)	Exposure-duration weighting factor	Arithmetic mean [L/(kg-d)]	Arithmetic standard deviation [L/(kg-d)]	Geometric mean [L/(kg-d)]	Geometric standard deviation [L/(kg-d)]
0 to 1	1/70 = 0.01428	0.0532	0.0509	0.0384	2.24
1 through 10	10/70 = 0.14286	0.0387	0.0238	0.0330	1.76
11 through 19	9/70 = 0.12857	0.0184	0.0107	0.0159	1.72
20 through 64	45/70 = 0.64286	0.0214	0.0122	0.0186	1.70
65 to 70	5/70 = 0.07143	0.0231	0.0097	0.0213	1.50
<i>All</i>	1.00000	0.0242	0.0170	0.0198	1.88

approximately lognormal and so the geometric mean and geometric standard deviation are calculated from the arithmetic mean (expected value) and arithmetic standard deviation reported by Ershow and Cantor (1989) (see bottom row of Table B-1; method for computing the geometric mean and geometric standard deviation from the arithmetic mean and arithmetic standard deviation of a lognormal distribution appears immediately after Eq. B-1, which is in next section of this appendix addressing air-inhalation rate). This geometric mean and geometric standard deviation can then be introduced into *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) computer software to construct the composite lognormal distribution. The composite distribution is the one needed for performing Monte-Carlo simulations to address exposure and risk for someone picked at random from the population with an exposure duration likely to be experienced by the population at risk. The 95th-percentile

upper-bound value for this approximately lognormal composite distribution of the ratio Ing can also easily be calculated from the geometric mean and geometric standard deviation appearing in the last row of Table B-1 (see Eq. B-1, which appears in the next section addressing air-inhalation rate).

The lifetime, TWA cdf for the ratio Ing is obtained by first constructing individual probability mass functions (pmfs) for each of the western-region age-group-specific distributions (see Table B-1). These distributions are considered approximately lognormal, so a geometric mean and geometric standard deviation for each age-group-specific distribution of Ing is derived from its respective arithmetic mean and arithmetic standard deviation reported by Ershow and Cantor (1989) (see Table B-1, and calculation procedure described after Eq. B-1 in next section addressing air-inhalation rate). Next, the geometric mean and geometric standard deviation for each age-group specific distribution is introduced into *Crystal Ball*[®], version 4.0 (Decisioneering, Inc., 1996) software in order to construct a corresponding age-group specific lognormal pmf. Then, the TWA cdf is obtained by performing the following procedure using *Crystal Ball*[®], version 4.0 (Decisioneering, Inc., 1996).

First, each of the age-specific lognormal pmfs is randomly sampled and each selected Ing is multiplied by its respective age-specific exposure-duration weighting factor (i.e., the applicable fraction of a 70-y lifetime, appearing in Table B-1). Following the sampling and weighting of each value, the weighted age-specific values are summed together to obtain a single lifetime, TWA value. This procedure is repeated 2000 times yielding 2000 equally likely TWA values. Because each of the 2000 TWA values are assumed to occur with equal probability, the expected value for the new TWA distribution is 2000^{-1} times the sum of the 2000 TWA values. To obtain the cdf from which the 95th-percentile upper bound is determined, the resulting 2000 TWA

values can be listed in a spreadsheet in increasing order with their corresponding probabilities, which are each equal to 1/2000. Then for each TWA value, the cumulative percentile value can be determined. As noted in the text, the expected value of this distribution is nearly equal to that of the composite distribution. The 95th-percentile upper bound value of *Ing* can be obtained directly from these listed values that describe the TWA cdf. As discussed in the text, this 95th-percentile upper-bound value of the TWA cdf is then used to obtain a deterministic estimate of the upper “conservative” bound for risk.

Inhalation rate of air [Inh; m³/(kg-d)]

The arithmetic mean and arithmetic standard deviation of the distribution of the ratio of age-specific inhalation rate to body weight was reported for California youth and adults in units of L/(kg-d) by OEHHA (1996) [based on an evaluation of data collected by Adams (1993) and Wiley et al. (1991a,b); according to a discussion with Marty (1998)]. These two age-specific distributions were identified as being lognormal. Accordingly, a geometric mean and geometric standard deviation can be determined for each age-group-specific distribution (see Table B-2), and spreadsheet software can be employed to construct from these values complete lognormal cdfs. The composite distribution for the ratio (*Inh*) of inhalation rate to body weight [m³/(kg-d)] is obtained from these cdfs using the respective age-specific population fractions as weighting factors. These weighting factors are represented by the age-adjusted population fractions shown in Table B-2, and they were determined from US Census Bureau data (USCB, 1998).

Table B-2. Weighting factors and age-specific ratios (*Inhs*) of inhalation rates to body weights [L/(kg-d) or m³/(kg-d)] used for constructing respective composite and lifetime, time-weighted-average (TWA) distributions [from Tables 3.19 and 3.20 in OEHHA (1996)]. To convert L/(kg-d) to units of m³/(kg-d), divide L/(kg-d) by 1000 L/m³.

Age (y)	Age-adjusted population fraction weighting factor ^a	Exposure-duration weighting factor	Arith-metic mean [L/(kg-d)]	Arith-metic standard deviation [L/(kg-d)]	Geo-metric mean [m ³ /(kg-d)]	Geo-metric standard deviation [m ³ /(kg-d)]
0 to 12	$\frac{46,618,155}{270,732,000} = 0.172193$	$12/70 = 0.17143$	452	67.73	0.4470	1.1607
12 to 70	$\frac{224,113,845}{270,732,000} = 0.827807$	$58/70 = 0.82857$	225.2	64.634	0.2165	1.3249

^a Age-adjusted weighting factor is obtained from population fraction for similar age categories of US population (USCB, 1998).

The procedure that is performed with spreadsheet software to construct this composite distribution for *Inh* begins by employing Eq. B-1 to estimate the value of *Inh* corresponding to intervals of 0.01 probability (i.e., between 0 and 1.0) for each of the two age-specific lognormal distributions (see Table B-2).

$$Inh_p = GM \times GSD^{z_p}, \text{ where} \quad (B-1)$$

Inh_p = daily inhalation rate per kg body weight [L/(kg-d)] for cumulative increments of probability, *p*, where each probability interval equals 0.01 for $0 \leq p \leq 1.00$;

GM = geometric mean of the distribution: $GM = (\mu^2) \times [(\mu^2) + (\tilde{\sigma}^2)]^{-0.5}$, where μ is the arithmetic mean and $\tilde{\sigma}$ is the arithmetic standard deviation of the parent distribution;

GSD = geometric standard deviation of the distribution: $GSD = \exp \{ \ln [1 + (\tilde{\sigma}^2 / \mu^2)] \}^{-0.5}$, where μ is the arithmetic mean and $\tilde{\sigma}$ is the arithmetic standard deviation of the parent distribution;

z_p = $\Phi^{-1}(p)$, where Φ is the cumulative standard normal distribution function.

Next, the computed values of *Inh* for both distributions are then combined together and listed in ascending order in one column of the spreadsheet. For each of these *Inh* values a cumulative probability is calculated for each age-group-specific distribution, and these results can be placed into two adjoining columns of the spreadsheet. The cumulative probability is obtained by rearranging the terms in Eq. B-1 so that the age-group-specific z score corresponding to each value of *Inh* is determined and the appropriate spreadsheet function can then be applied to determine the corresponding cumulative probability for that age-group-specific z score. The cumulative probability in each age-group-specific distribution, which corresponds to the same value of *Inh*, is then multiplied by its applicable weighting factor represented by the age-adjusted fraction of the population. These products from each age-group-specific distribution are summed together to obtain a weighted average of cumulative probability that corresponds to each value of the ratio *Inh*. The resulting list of 100 paired (*Inh* and weighted-average cumulative probability) values is the composite cdf that can be introduced into *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software for performing Monte-Carlo simulations to address someone picked at random from the population with an exposure duration likely to be experienced by the population at risk.

The TWA cdf is obtained by performing the following procedure using *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software. First, the pmfs for each age-specific lognormal distribution are created using the geometric means and geometric standard deviations of these distributions (from Table B-2) in *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software. Then, the TWA cdf is obtained by performing the following procedure using *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996).

First, each of the age-specific lognormal pmfs is randomly sampled and each selected *Inh* is multiplied by its respective age-specific exposure-duration weighting factor (i.e., applicable fraction of a 70-y lifetime, appearing in Table B-2). Following the sampling and weighting of each value, the (two, in this case) weighted age-specific values are summed together to obtain a single lifetime, TWA value. This procedure is repeated 2000 time so that 2000 equally likely TWA values are obtained. Because each of the 2000 TWA values are assumed to occur with equal probability, the expected value for the new TWA distribution is 2000^{-1} times the sum of the 2000 TWA values. As noted in the text, the expected value of this distribution is equal to that of the composite distribution. To obtain the cdf from which the 95th-percentile upper bound is determined, the resulting 2000 TWA values can be listed in a spreadsheet in increasing order with their corresponding probabilities, which are each equal to 1/2000. Then for each TWA value, the cumulative percentile value can be determined and assigned. The 95th-percentile upper bound value of the ratio of inhalation rate to body weight can be obtained directly from these listed values that describe the TWA cdf. As discussed in the text, this 95th-percentile upper-bound value of the TWA cdf is then used to obtain a deterministic estimate of the upper “conservative” bound for risk.

Surface area per kg body weight [A; cm²/(kg d)]

The composite distribution for the ratio (A) of surface area to body weight (cm²/kg) is constructed from data for three age-specific empirical distributions provided by Phillips et al. (1993) that appears in Table B-3. The procedure followed involves the following steps. First, all of the values of A from all three distributions are

Table B-3. Weighting factors and age-specific ratios (As) of surface areas to body weights (cm²/kg) used for constructing respective composite and lifetime, time-weighted-average (TWA) distributions [from Table 4 in Phillips et al. (1993)].

Age-group (y)	Age-adjusted population fraction weighting factor ^a	Exposure-duration weighting factor	Percentile of age-group empirical distributions and corresponding surface area to body weight ratio (cm ² /kg)							
			0	5	10	25	50	75	90	95
0 to 2	$\frac{7,593,200}{270,732,000} = 0.028047$	$2/70 = 0.02857$	421	470	507	563	617	719	784	846
2 to 18	$\frac{62,239,800}{270,732,000} = 0.229894$	$16/70 = 0.22857$	268	291	328	376	422	454	501	594
≥ 18	$\frac{200,899,000}{270,732,000} = 0.742059$	$52/70 = 0.74286$	200	238	244	270	286	302	316	329

^a Age-adjusted weighting factor is obtained from population fraction for similar age categories of US population (USCB, 1998).

listed together in a spreadsheet and then sorted into ascending order. Then, for each age-specific group, the probability for each of the surface area to body weight ratios is assigned based on the data reported in Table B-3 for the specific age-group, or in the absence of a reported value, the value is computed by linear interpolation using Eq. B-2.

$$P_i = P_1 + \left[\left(\frac{a_i - a_1}{a_2 - a_1} \right) \times (P_2 - P_1) \right], \text{ where} \quad (\text{B-2})$$

P_i = probability (expressed as decimal) corresponding to the surface area to body weight ratio of interest (i.e., a_i ; cm²/kg);

P_1 = probability (expressed as decimal) associated with the surface area to body weight ratio that is just less than the one of interest and for which probability is known or has been calculated (i.e., a_1);

- P_2 = probability (expressed as decimal) associated with surface area to body weight ratio that is just greater than the one of interest and for which probability is reported (i.e., a_2);
- a_i = surface area to body weight ratio of interest (cm^2/kg);
- a_1 = surface area to body weight ratio that is just less than the one of interest and for which a probability value is reported or has been calculated (cm^2/kg); and
- a_2 = surface area to body weight ratio that is just greater than the one of interest and for which a probability value is reported (cm^2/kg).

For example, for age-group 0 to 2 y the values of A from 200 to 421 cm^2/kg all have probabilities equal to zero, and 422 cm^2/kg is the first value of interest in that age group that is calculated by linear interpolation. This calculation is performed by substituting into Eq. B-2 values of A equal to 422, 421, and 470 cm^2/kg for terms a_i , a_1 , and a_2 , respectively, and the corresponding probabilities for 421 and 470 cm^2/kg for this age group for terms P_1 and P_2 , respectively (i.e., 0 and 0.05), from Table B-3.

Similarly, for the age-group from 2 to 18 y the values of A from 200 to 268 cm^2/kg all have probabilities equal to zero, and 270 cm^2/kg is the first value in that age group that is calculated by linear interpolation. In this case, values of A equal to 270, 268, and 291 cm^2/kg are substituted into Eq. B-2 for terms a_i , a_1 and a_2 , respectively, along with the corresponding probabilities for 268 and 291 cm^2/kg for this age group (see Table B-3) to represent terms P_1 and P_2 , respectively (i.e., 0 and 0.05). A final example is for the last age group (≥ 18 y), where only 200 cm^2/kg has a probability equal to zero, and the first value of A to have its probability determined by linear interpolation is 268 cm^2/kg . In this last case, values of A equal to 268, 244, and 270 cm^2/kg are substituted into Eq. B-2 for terms a_i , a_1 and a_2 , respectively, along with corresponding probabilities for 244 and 270 cm^2/kg for this age group (see Table B-3) that represent terms P_1 and

P_2 , respectively (i.e., 0.10 and 0.25). This process is repeated in each age-group for values of A for which interpolation must be performed.

The next step is to weight each age-group-specific cumulative probability that is associated with a particular value of A by its appropriate age-adjusted population fraction (see Table B-3). Then, for each value of A , the sum of the products of age-group-specific cumulative probabilities and applicable weighting factors equates to a weighted functional average cumulative probability. These resulting paired values of A and corresponding weighted cumulative probabilities represent the composite cdf that can be inserted into *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software for performing Monte-Carlo simulations to address someone picked at random from the population with an exposure duration likely to be experienced by the population at risk.

As was done for *Ing* and *Inh*, the TWA cdf for A is obtained by performing the following procedure using *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software. First, the empirical cdfs reported by Phillips et al. (1993) are introduced into *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software (in their cumulative form) and randomly sampled. The value A from each distribution is then randomly sampled and multiplied by its respective age-specific exposure-duration weighting factor (i.e., applicable fraction of a 70-y lifetime, appearing in Table B-3). All of these weighted age-specific values are then summed to obtain a single TWA value. Then, this procedure is repeated 2000 times. Because each of the 2000 TWA values are assumed to occur with equal probability, the expected value for the new TWA distribution is 2000^{-1} times the sum of the 2000 TWA values. As noted in the text, the expected value of this distribution is equal to that of the composite distribution. To obtain the cdf from which the 95th-percentile upper bound is determined, the resulting 2000 TWA values can be listed in a spreadsheet in increasing order with their corresponding probabilities, which

are each equal to 1/2000. Then for each TWA value, the cumulative percentile value can be determined and assigned. The 95th-percentile upper bound value of the ratio of A can be obtained directly from these listed values that describe the TWA cdf. As discussed in the text, this 95th-percentile upper-bound value of the TWA cdf is then used to obtain a deterministic estimate of the upper “conservative” bound for risk.

Constructing the Student’s T distribution for Applicable Degrees of Freedom

The Student’s T distribution for the applicable degrees of freedom ($n - 1$, where n is the number of available sample values) is easily constructed using spreadsheet software and an “inverse” Student’s T function. The process followed involves listing very small equal intervals (e.g. ≤ 0.0025) in ascending order of cumulative probabilities between 0 and 1.0. Then for each cumulative probability, the value of the Student’s T distribution is identified using the inverse Student’s T distribution function with the applicable number of degrees of freedom. For the three reported concentrations of TCE in water (Purrier, 1997), the Student’s T distribution has 2 degrees of freedom. For the 14 reported values of water-to-air transfer efficiency for showers running water at temperatures ≥ 30 °C (Corsi and Howard, 1998), the corresponding Student’s T distribution has 13 degrees of freedom. These Student’s T distributions are then inserted into *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software, and used in performing Monte-Carlo simulations of the mean concentration of TCE in ground water (Eq. 4 in text), and the water-to-air transfer efficiency of TCE in shower water (Eq. 5 in text).

Constructing Distributions for Exposure Duration (i.e., Residence Time)

The conservative approximation for the 95th percentile upper-bound of exposure duration (i.e., residence time), \hat{ED} , which is used to compute \hat{R}_{High} , equals 55.28 y. This upper-bound value reflects variability in total time of residence and is obtained directly by linear interpolation of the cumulative probability distribution for $1 - R(t)^{f_m^*}$. This distribution is constructed by solving for $R(t)^{f_m^*}$ for time (t) ranging from 0 to 70 y, in one year increments, and assigning f_m^* (i.e., fraction of moves outside the water supply district) the value equal to 0.439, which is the 5th percentile of its triangular distribution that ranges from 1/3 to 1 with a mode at 2/3 (see also Eqs. 8 and 11 and Table 1 in this text]. The equation for $R(t)$ is from Israeli and Nelson (1992) and is shown as Eq. B-3.

$$R(t) = \frac{e^{-\left[a_1 b_1 \left(1 - e^{-\frac{t}{b_1}} \right) + a_2 t + a_3 b_3 \left(e^{\frac{t}{b_3}} - 1 \right) \right]}}{a_1 + a_2 + a_3} \left(a_1 e^{-\frac{t}{b_1}} + a_2 + a_3 e^{-\frac{t}{b_3}} \right), \text{ where} \quad (\text{B-3})$$

t equals time and the terms a_1 , b_1 , a_2 , a_3 , and b_3 are nonnegative parameters equal to values of 0.2029, 1.74, 0.0832, 0.008, and 10.3, respectively, for the western region of the US (as determined and presented by Israeli and Nelson, 1992).

The distribution for the population-average value of total residence time, \overline{ED} , is constructed using the following procedure. First, an approximate solution is obtained for the integral shown in Eq. 10 in text based on 2000 equal intervals of time (t) between 0 and 70 y (i.e., increments = 70/2000 or 0.035 y), and a specific value of f_m selected at random from its triangular distribution using *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software. For example,

$$\overline{ED}_j \approx \Delta t \left[\sum_{i=2}^{n-1} y_i + \left(\frac{y_1 + y_n}{2} \right) \right] \quad \text{by linear approximation (the "trapezoidal rule"),} \quad (\text{B-4})$$

where $n = 2000$ equal intervals of time between 0 and 70 y, $y_i = R(t_i)^{f_m}$ at an i th increment of time corresponding to a specific interval of 0.035 y from 0 to 70 y, and any j th value of f_m selected at random from its triangular distribution using *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software. For odd values of n (e.g., 2001), a better parabolic, approximation (Simpson's Rule) may be used:

$$\overline{ED}_j \approx \frac{\Delta t}{3} \left[y_1 + 2 \left(\sum_{i=1}^{\frac{n-3}{2}} 2y_{2i} + y_{2i+1} \right) + 4y_{n-1} + y_n \right] \quad (\text{B-5})$$

In either case, the process is then repeated for $n - 1$ more randomly selected j th values of f_m . The resulting n values of \overline{ED} are then listed in ascending order, and assigned a cumulative probability based on each value being assumed to occur with an equal likelihood of 1/2000 (or 0.0005). The expected value for this distribution (in this case approximately 7.6 y) is therefore the sum of the \overline{ED} values divided by 2000. This cdf is then used for Monte-Carlo simulations requiring \overline{ED} . However, note that only about 400 paired values for any distribution can be inserted into *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software to create a distribution for sampling. Therefore, the cdf in the spreadsheet must be reduced in size and described by only 400 equal probability intervals of 0.0025, which can be selected from the listed values. The 95th-percentile upper bound for this distribution can be obtained from the listed values for the cdf.

The distribution of the cumulative probability reflecting variability in total time of residence, $\langle ED \rangle$, is obtained using Eq. 12 in the text, with time (t) increasing in intervals of 0.1 y from 0 to 10 y, increasing in intervals of 1 y from 11 to 50 y, and increasing in intervals of 5 years from 55 to 70 y. This list of time vs. probability values is then used in *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software for performing Monte-Carlo simulations. The expected value and 95th percentile upper bound for this distribution are obtained by using *Crystal Ball*®, version 4.0 (Decisioneering, Inc., 1996) software to perform a Monte-Carlo simulation involving 2000 or more trials and having it report the expected (mean) and 95th-percentile upper-bound values for the resulting distribution.

Exposure and Traditional Risk-Related (point) Estimators

The input parameters, corresponding values, and respective resulting deterministically calculated exposure (E_{Ing} , E_{Inh} , and E_{Derm}) and traditional risk-related (\hat{R}_E , “best” estimate; \hat{R}_{RME} , risk to “reasonably maximum exposed” person; and \hat{R}_{High} , upper “conservative” bound) (point) estimators are presented in Table B-4. The purpose of Table B-4 is to summarize the specific inputs and outputs associated with deterministically calculating these exposure and traditional risk-related estimators using Eqs. 1 through 3 and Eq. 13 in the text.

Determining P_0 Using Simulated \bar{R} Values

The probability, P_0 , that there will be no additional cases of cancer in a given population, n_T , over a 70-y period, is approximated as follows. First, 2000 values of \bar{R} are generated using a Monte-Carlo simulation of 2000 trials. A corresponding

Table B-4. Input parameters, corresponding values, and respective resulting deterministically calculated exposure (E_{Ing} , E_{Inh} , and E_{Derm}) and traditional risk-related (\hat{R}_E , “best” estimate; \hat{R}_{RME} , risk to “reasonably maximum exposed” person; and \hat{R}_{High} , upper “conservative” bound) (point) estimators.

Inputs and corresponding estimates of exposure and risk ^a	Distribution represents ^b	Related to \hat{R}_E ^c	Related to \hat{R}_{RME} ^d	Related to \hat{R}_{High} ^e
EF (d/y)	NA (constant)	350	350	350
AT (d in 70-y lifespan)	NA (constant)	25,550	25,550	25,550
ED (y)	JUV	7.6 ^f	30 ^g	55.3 ^h
C_w (mg/L)	Uncertainty	0.0223	0.0223	0.0301
Ing (L/kg-d)	Variability	0.0242	0.0286 ^g	0.0399
E_{Ing} [mg/kg-d]	NA	5.6×10^{-5}	2.6×10^{-4}	9.1×10^{-4}
CSF_{Ing} [R/[mg/(kg-d)]]	NA (constant)	0.015	0.015	0.015
Traditional risk-related (point) estimators for ingestion pathway	NA	8.4×10^{-7}	3.9×10^{-6}	1.4×10^{-5}
EF (d/y)	NA (constant)	350	350	350
AT (d in 70-y lifespan)	NA (constant)	25,550	25,550	25,550
ED (y)	JUV	7.6 ^f	30 ^g	55.3 ^h
C_w (mg/L)	Uncertainty	0.0223	0.0223	0.0301
Inh [m ³ /(kg-d)]	Variability	0.264	0.286 ^g	0.363
W_{sh} and W_{b} (L/h)	Variability	480	777	777
W_{h} (L/h)	Variability	42	69.9	69.9
$\phi_{\text{TCE-sh}}$ (dimensionless)	Variability	0.76	0.81	0.81
$\phi_{\text{TCE-h}}$ (dimensionless) ⁱ	Variability	0.59	0.63	0.63
AE_{sh} (m ³ /h)	Variability	9.94	4.82	4.82
AE_{b} (m ³ /h)	Variability	39.1	14.6	14.6
AE_{h} (m ³ /h)	Variability	649	344	344

Table B-4 (continued).

Inputs and corresponding estimates of exposure and risk ^a	Distribution represents ^b	Related to \hat{R}_E^c	Related to \hat{R}_{RME}^d	Related to \hat{R}_{High}^e
ET_{sh} (h/d)	Variability	0.129	0.13 ^g	0.226
ET_b (h/d)	Variability	0.330	0.744	0.744
ET_b (h/d)	Variability	14	16.4 ^g	19.4
D (h/d) ^j	NA (constant)	24	24	24
E_{inh} [mg/kg-d]	NA	2.1×10^{-4}	5.6×10^{-3}	2.2×10^{-2}
CSF_{Ing} {R/[mg/(kg-d)]}	NA (constant)	0.010	0.010	0.010
Traditional risk-related (point) estimators for inhalation pathway	NA	2.1×10^{-6}	5.6×10^{-5}	2.2×10^{-4}
EF (d/y)	NA (constant)	350	350	350
AT (d in 70-y lifespan)	NA (constant)	25,550	25,550	25,550
ED (y)	JUV	7.6 ^f	30 ^g	55.3 ^h
C_w (mg/L)	Uncertainty	0.0223	0.0223	0.0301
ϕ_{TCE-sh} (dimensionless)	Variability	0.76	0.81	0.81
A (cm ² /kg)	Variability	326	329 ^g	373
f_s (dimensionless)	Variability	0.65	0.875	0.875
k_p (cm/h)	Variability	0.263	0.293	0.293
ET_{sh} (h/d)	Variability	0.129	0.13 ^g	0.226
cf (L/cm ³) ^k	Constant	0.001	0.001	0.001
E_{Derm} [mg/kg-d]	NA	1.0×10^{-5}	6.0×10^{-5}	2.9×10^{-4}
CSF_{Derm} {R/[mg/(kg-d)]} ^l	NA (constant)	0.015	0.015	0.015
Traditional risk-related (point) estimators for dermal absorption pathway	NA	1.5×10^{-7}	9.0×10^{-7}	4.4×10^{-6}

Table B-4 (continued).

Inputs and corresponding estimates of exposure and risk ^a	Distribution represents ^b	Related to \hat{R}_E ^c	Related to \hat{R}_{RME} ^d	Related to \hat{R}_{High} ^e
<i>Total for traditional risk-related estimators (i.e., sum for all pathways)^m</i>	NA	3.1×10^{-6}	6.1×10^{-5}	2.4×10^{-4}

^a Symbols are defined in Table 1 and/or Eqs. 1 through 3 in text.

^b From Table 1 and/or Eqs. 1 through 3 in text; NA = not applicable with respect to a distribution representation because value is either a constant or a deterministically calculated point estimate.

^c Expected values (from Table 1 in text) are used for variates (and similarly for the calculations of $\langle \bar{R} \rangle$ and $\langle \bar{R} \rangle$ using exact expressions).

^d As noted in footnote to Table 2 in text: if available, regulatory default values (see data in Table 2 in text) are used for variates; otherwise, expected values (from Table 1 in text) are used for uncertain variates and 95th-percentile upper-bound values (from Table 1 in text) are used for heterogeneous ones (or in the case of air-exchange rates only, and for reasons explained in footnote "c" of Table 1 in text, the 5th-percentile values are used).

^e The 95th-percentile upper-bound values (from Table 1 in text) are used for variates (or in the case of air-exchange rates only, and for reasons explained in footnote "c" of Table 1 in text, the 5th-percentile values are used).

^f This expected value is discussed in this appendix and also mentioned in the footnote to Table 4 in text.

^g Regulatory value (based on data presented in Table 2 in text).

^h Approximation for 95th-percentile upper-bound of exposure duration, \hat{ED} [see explanation in this appendix; and see also Eqs. 8 and 11 and Table 1 in text].

ⁱ Calculation of term explained after Eq. 2 in text.

^j Term is described after Eq. 2 in text.

^k Term is described after Eq. 3 in text.

^l For purposes of this analysis the ingestion cancer slope factor (CSF_{Ing}) is also considered to apply to dermal absorption (CSF_{Derm}), based on regulatory guidance (see Eq. 13 and discussion that follows in text, and Tables 1 and 2 in text).

^m These totals for the traditional risk-related (point) estimators are listed in Table 3 in text. (The values for exposure intakes: E_{Ing} , E_{Inh} , and E_{Derm} , are not presented in text.)

value of $e^{-n_T \bar{R}}$ is computed for each of the 2000 \bar{R} values conditional on a specific total population size n_T (see Table 4 in text). Because each of these values is assumed to have an equal probability of occurrence of $1/2000$ (i.e., 0.0005), the 2000 values of $e^{-n_T \bar{R}}$ can be summed and multiplied by $1/2000$ to obtain a value for P_0 , which is the solution to the integral shown in Eq. 18 in text. Repeating this process 10 times for each value of n_T makes it possible to obtain a mean value and to compute a CVM (in percent) for a P_0 and value of n_T . As explained in the text, the value of $1 - P_0$ represents the probability that for a given population n_T there will be one or more (i.e., more than zero) additional cases of cancer (i.e., the probability that $N \geq 1$). The expected number of cases is defined as $\langle N \rangle = n_T \times \langle \bar{R} \rangle$, which is not necessarily an integer.

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